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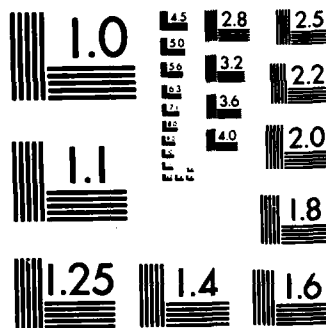
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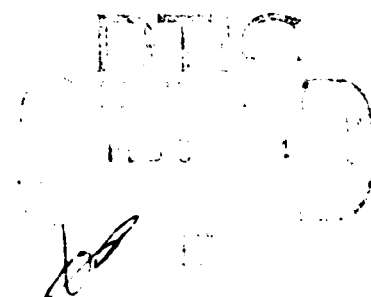
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# AFRRI TECHNICAL REPORT

**Spectrum-averaged kerma factors  
for reactor dosimetry with paired  
ion chambers**

**K. P. Ferlic  
G. H. Zeman**



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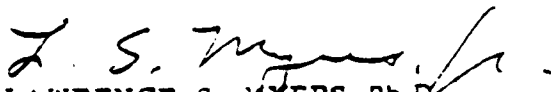
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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) Neutron and gamma spectrum-averaged kerma factors (SAKF's) were calculated for four reference spectra and 18 configurations of the AFRRI TRIGA reactor for materials of interest in dosimetry applications. Reactor gamma SAKF ratios for tissue to carbon and for tissue to magnesium (ion chamber wall materials) gave average values $\pm 2$ standard deviations of $1.13 \pm 1\%$ and $1.09 \pm 3\%$ , respectively. For some reactor configurations, the gamma SAKF ratios were as much as 7.6% different from corresponding values for		

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20. ABSTRACT (continued)

→ cobalt-60 gamma rays. Reactor neutron SAKF ratios for ICRU (International Commission on Radiation Units and Measurements) muscle to ion chamber gas materials were as follows: TE (tissue-equivalent) gas,  $0.983 \pm 0.5\%$  for all configurations; carbon dioxide,  $9.8 \pm 10\%$ ; and argon,  $71 \pm 27\%$ . At depth in a phantom, the neutron SAKF for ICRU muscle differed substantially from the free-in-air value for the same reactor configuration. This finding suggests the need for more thorough spectrum determinations in anatomical phantoms and for more sophisticated dosimetric tools to better quantitate the dose deposition process.

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## INTRODUCTION

Kerma (kinetic energy released in material) is defined as the amount of energy per unit mass transferred by indirectly ionizing radiation to charged particles in a volume of material. Kerma is equal to radiation-absorbed dose under conditions of charged particle equilibrium, provided that energy loss due to bremsstrahlung is negligible. Kerma factors [expressed in units of rad per unit radiation fluence ( $\text{rad} \cdot \text{cm}^2$ )] are functions of the radiation type (neutrons or gamma rays), radiation energy, and material irradiated. Kerma factors are used in neutron gamma dosimetry for a reactor to calculate radiation dose when the fluence is known. Ratios of kerma factors are used to calculate radiation dose in one material, such as tissue, when the radiation dose is known or has been measured in another material, such as an ion chamber (1).

Irradiation by neutrons or gamma rays of a spectrum of energies requires the use of spectrum-averaged kerma factors (SAKF's) to perform dosimetry calculations. Detailed energy spectra were recently determined (2,3) for several configurations of the AFRRI TRIGA reactor. These spectra were used in the present report to calculate SAKF's and ratios of SAKF's for the following materials of interest in reactor neutron gamma dosimetry with paired ion chambers:

$(K_T)_G, (K_T)_N$	Gamma and neutron SAKF's for tissue
$(K_T/K_C)_G, (K_T/K_{Mg})_G$	Gamma SAKF ratios for carbon and magnesium (ion chamber wall materials)
$(K_T/K_{Ar})_N, (K_T/K_{CO_2})_N,$ and $(K_T/K_{TE \text{ gas}})_N$	Neutron SAKF ratios for argon, carbon dioxide, and tissue-equivalent (TE) gas (ion chamber gases)

## METHODS

### Neutron and Gamma Spectra

Neutron and gamma spectra for 18 configurations of the AFRRI TRIGA reactor have been reported (2,3). Table 1 summarizes the configurations for which spectra are available, and Figure 1 shows two sample spectra. The spectra were reported in the format of Oak Ridge Data Library Collection DLC-31 (4), which consists of a 37-energy-group format for neutron spectra and a 21-energy-group format for gamma spectra. Angular distributions of the neutrons were reported in terms of "front" and "back" directions of incidence, but only the total ("front" plus "back") spectra were used in the calculations presented here.



Table 1. Reactor Configurations for Neutron and Gamma Spectra

Room	Distance to Core (cm)	Configuration	Average Energy (MeV)		Neutron Spectra *
			Neutron	Gamma	
1	50	Unshielded	1.46	1.16	1-D
	100	Unshielded	1.49	1.15	1-D, 3-D, MEAS
	200	Unshielded	1.32	1.05	1-D
	300	Unshielded	1.16	0.91	1-D
	400	Unshielded	1.11	0.78	1-D
	500	Unshielded	0.89	0.67	1-D
2	50	Unshielded	1.35	1.18	1-D
	100	Unshielded	1.32	1.13	1-D, 3-D, MEAS
	200	Unshielded	1.12	0.95	1-D
	300	Unshielded	0.93	0.76	1-D
NA	NA	Pneumatic tubes	0.88	0.83	1-D
1	100	7.5 cm H <sub>2</sub> O	1.99	1.04	1-D
	100	30 cm H <sub>2</sub> O	3.71	0.95	1-D, 3-D
	100	5 cm Pb	1.58	1.65	1-D, 3-D
	100	5 cm Pb and exercise wheel	1.05	1.36	1-D, 3-D, MEAS
	100	15 cm Pb	0.96	0.92	1-D, 3-D
	100	15 cm Pb and cave	0.68	1.80	1-D, 3-D, MEAS
	100	15 cm Pb and cylindrical phantom	0.55	1.13	1-D, 3-D, MEAS

\* 1-D, 3-D, and MEAS refer to the availability of neutron spectral data derived from one-dimensional ANISN calculations, three-dimensional Monte Carlo calculations, or activation foil measurements, respectively (2,3).

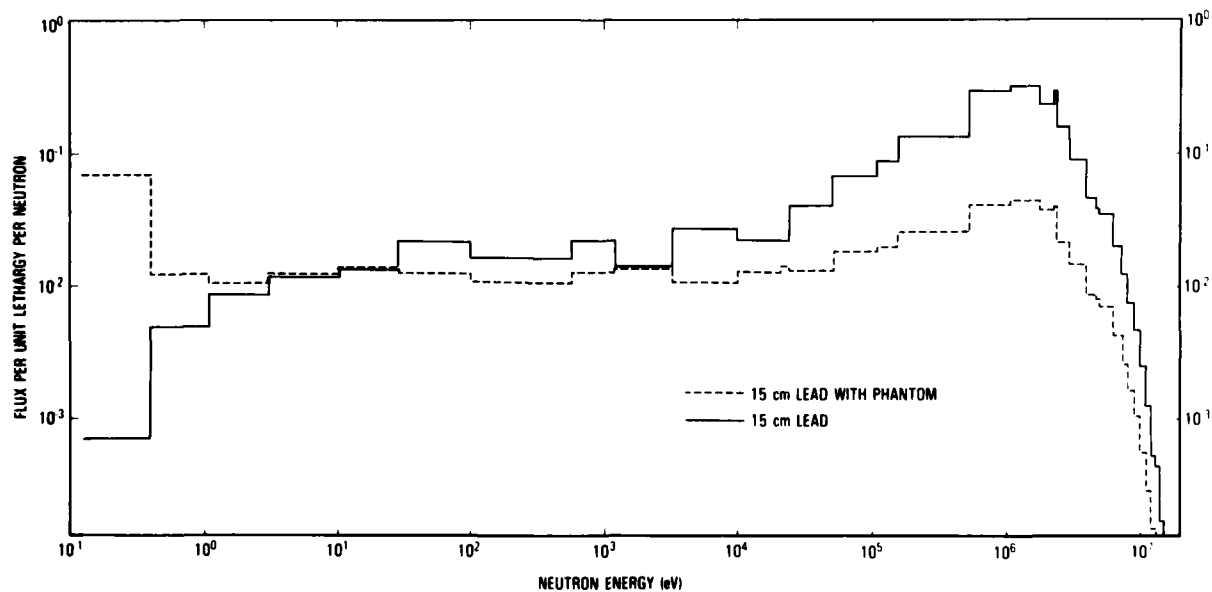


Figure 1. Neutron spectra at 100 cm from the AFRRI TRIGA reactor, shielded by 15-cm lead wall. Solid curve shows spectrum free in air; dashed curve shows spectrum at midline in an 18-cm-diameter cylindrical tissue-equivalent phantom.

The focus of the spectrum calculations of references 2 and 3 was on neutron spectra; thus more reliance can be placed on these than on the gamma spectra. In all cases, one dimensional (1-D) ANISN calculations of the spectra were performed. The gamma spectra excluded fission and fission-product gamma radiation since secondary gamma rays were presumed to dominate the spectrum (3). Therefore, the shapes of the gamma spectra (which depend on the materials irradiated) are probably realistic, but the absolute magnitudes (which depend on the calculational model) must be viewed with caution. For the neutron spectra, the calculations were refined with three-dimensional (3-D) MORSE calculations in nine cases, and verified by activation foil measurements in five of the more complex cases. Thus the neutron spectra represent the best state-of-the-art determinations now available.

To indicate the degree of moderation of each neutron and gamma spectrum, average spectrum energies were computed according to the following formula (and are listed in Table 1):

$$E_{avg} = \frac{\int_{0.4 \text{ eV}}^{\infty} E \Phi(E) dE}{\int_{0.4 \text{ eV}}^{\infty} \Phi(E) dE} = \frac{\sum_{i=1}^{21 \text{ or } 36} E_i \phi_i \Delta E_i}{\sum_{i=1}^{21 \text{ or } 36} \phi_i \Delta E_i} \quad \text{Eq. 1}$$

where  $E$  and  $E_i$  represent neutron or gamma ray energy, and  $\phi(E)$  and  $\phi_i$  represent the number of neutrons or gamma rays with that energy. Note that this definition of average energy excludes thermal neutrons.

In addition to the spectra listed in Table 1, SAKF's were also calculated for the reference spectra given in DLC-31 (4). These spectra were prompt gamma-ray fission source, neutron spectra for fission and thermonuclear sources, and 14-MeV neutrons. A final reference spectrum was the ENDF uranium-235 fission spectrum, which was used as the source term for the AFRRI neutron spectrum calculations (2). While none of these spectra apply directly to the AFRRI reactor configurations, they were included in the present calculations for comparison purposes.

#### Gamma Kerma Factors

Gamma kerma factors for tissue in a 21-group format were taken directly from DLC-31 (4). Although DLC-31 tissue represents a standard man composed of 11 elements, the gamma kerma factors compared reasonably well with those calculated from mass energy transfer coefficients for muscle (5). Gamma kerma factors for the elements carbon and magnesium (ion chamber wall materials) were also taken directly from DLC-31 (4).

## Neutron Kerma Factors

In addition to gamma kerma factors, selected neutron kerma factors were contained in DLC-31 (4), but some materials of particular interest for paired ion chamber constants were not covered, namely ICRU muscle, muscle-equivalent gas, and argon. Consequently, the more complete neutron kerma factor data of ICRU Report 26 (1) were the basis for the present calculations. The energy grouping of the ICRU-26 kerma factor data did not match the 37-group structure of the neutron spectra, so restructuring of the groups was required. The procedures used to convert the ICRU-26 kerma factor data to the 37-group format are described in reference 6.

## Calculations

Spectrum-averaging calculations for neutron and gamma kerma factors were done with the AFRRI PDP11 computer. All kerma factor data and all neutron and gamma energy spectra were stored in formatted input files. A fortran computer program named SPT was written to complete the calculations and store the results in separate output files. SPT calculated the following quantities:

$$\text{SAKF} = \frac{\int_0^{\infty} K(E) \Phi(E) dE}{\int_0^{\infty} \Phi(E) dE} = \frac{\sum_{i=1}^{21 \text{ or } 37} K_i \Phi_i \Delta E_i}{\sum_{i=1}^{21 \text{ or } 37} \Phi_i \Delta E_i} \quad \text{Eq. 2}$$

where SAKF is the spectrum averaged kerma factor,  $K(E)$  and  $K_i$  are the energy-dependent kerma factors,  $\phi(E)$  and  $\phi_i$  are the neutron or gamma fluence, and  $E$  is the energy. Note that the SAKF integrals include thermal neutrons in the averaging process. A listing of SPT is contained in Appendix A.

## RESULTS

### Reactor Gamma SAKF

Gamma SAKF's for tissue are shown in Table 2. The difference between the gamma SAKF's for tissue for the various reactor configurations can be interpreted as changes in the effective energy of the gamma spectra. Tissue-effective energies of the gamma spectra given in Table 2 represent the single photon energies that would give the same tissue kerma factors as the gamma spectra in question. Tissue-effective gamma energies ranged from 0.6 to 1.5 MeV for the reactor configurations, and the energies correlate reasonably

well with the average energies of the spectra listed in Table 1. The fact that tissue-effective gamma energies were 0.1 to 0.3 MeV lower than spectrum-averaged energies expresses the higher attenuation coefficients of lower energy gamma rays in tissue. For materials other than tissue, the effective gamma energies could vary because of differences in atomic number.

Table 2. Reactor Gamma Spectrum-Averaged Kerma Factors and Ratios\*

Room	Distance to Core (cm)	Configuration	MeV <sub>eff</sub> (tissue)	(K <sub>T</sub> ) <sub>G</sub>	(K <sub>T</sub> /K <sub>C</sub> ) <sub>G</sub>	(K <sub>T</sub> /K <sub>Mg</sub> ) <sub>G</sub>
1	50	Unshielded	1.0	4.92	1.128	1.108
	100	Unshielded	1.0	4.88	1.130	1.107
	200	Unshielded	0.9	4.47	1.132	1.101
	300	Unshielded	0.8	3.89	1.134	1.090
	400	Unshielded	0.7	3.35	1.139	1.073
	500	Unshielded	0.6	2.93	1.149	1.054
2	50	Unshielded	1.0	5.00	1.129	1.109
	100	Unshielded	1.0	4.89	1.129	1.106
	200	Unshielded	0.8	4.04	1.135	1.092
	300	Unshielded	0.6	3.29	1.142	1.068
NA	NA	Pneumatic tubes	0.7	3.54	1.138	1.089
1	100	7.5 cm H <sub>2</sub> O	0.9	4.40	1.131	1.103
	100	30 cm H <sub>2</sub> O	0.8	3.99	1.137	1.093
	100	5 cm Pb	1.5	6.77	1.128	1.110
	100	5 cm Pb and exercise wheel	1.2	5.63	1.131	1.108
	100	15 cm Pb	0.8	3.93	1.142	1.082
	100	15 cm Pb and cave	1.5	6.70	1.132	1.076
	100	15 cm Pb and cylindrical phantom	1.0	4.74	1.133	1.092
	<u>Reference Spectra</u>					
	DLC-31	Prompt gamma ray fission	0.8	4.23	1.146	1.065
	Cobalt-60		1.25	5.98	1.126	1.134

\* (K<sub>T</sub>)<sub>G</sub> units are 10<sup>-10</sup> rad · cm<sup>2</sup>. (K<sub>T</sub>/K<sub>C</sub>) and (K<sub>T</sub>/K<sub>Mg</sub>) are ratios of SAKF's.

Also shown in Table 2 are the ratios of SAKF's for tissue to those for carbon and magnesium. The C and Mg data are presented in this format to be directly useful in dosimetry applications. Average values ( $\pm 2$  standard deviations) for C and Mg SAKF ratios for all reactor configurations are given below.

$$(K_T/K_C)_G = 1.133 \pm 1.0\%$$

$$(K_T/K_{Mg})_G = 1.09 \pm 3.1\%$$

Eq. 3

Corresponding kerma factor ratios for cobalt-60 gamma rays (1.25 MeV effective energy) are also shown in Table 2. For C, cobalt-60 gamma rays give a kerma factor ratio lower than for any of the reactor configurations; for Mg, it is higher. This finding is consistent with the presence of low-energy photons (below 300 keV) in each of the gamma spectra of the reactor configurations. The average values (Equation 3) for C and Mg gamma SAKF ratios differ by less than 4% from the corresponding ratios for cobalt-60. However, for some configurations, the influence of low-energy gamma rays is more pronounced and causes gamma SAKF ratios to differ from cobalt-60 values by up to 7.6%. This is the case at great distances from the reactor, where low-energy gamma rays arising from the walls exert an increasing effect, and also behind the 15-cm lead shield, where lead X rays presumably contribute to the total gamma-ray spectrum. On the other hand, the 5-cm lead shield appears to have a hardening effect on the gamma spectrum, as far as C and Mg gamma SAKF ratios are concerned.

#### Reactor Neutron SAKF for Tissue

Neutron spectra calculated from 3-D models are more reliable than those obtained from 1-D models. Consequently, the present calculations used 3-D neutron spectra for all reactor configurations for which they were available (see Table 1). Comparison of SAKF's for ICRU muscle obtained from 1-D and 3-D spectra is shown in Table 3 for those configurations for which both were available. For noncomplicated configurations such as unshielded at a distance of 100 cm, close agreement occurs between the 1-D and 3-D results. This agreement confirms the adequacy of the 1-D spectra for SAKF calculations at the other unshielded distances. Likewise, the reasonable agreement between the 1-D and 3-D results for the reactor shielded by 30 cm of water justifies the use of a 1-D spectrum for the 7.5-cm water shield. On the other hand, the lack of a 3-D spectrum for the pneumatic tubes leaves open the question of the adequacy of the 1-D neutron spectrum at that location.

Table 3 also presents SAKF values for ICRU muscle for the five measured neutron spectra. These values differ by 2%-58% from those determined from the 3-D calculated spectra. The closest agreement is for the lead cave configuration, for which the calculated and measured neutron spectra plotted in reference 3 are nearly coincident. For the worst case, the cylindrical phantom, the spectrum plots show a clear excess of neutrons below 300 keV in the calculated spectrum. Reference 3 explains this as being due to shortcomings in the calculated spectrum, on the assumption that the measured neutron spectrum is the more accurate. Thus, the SAKF differences between the 3-D and measured spectra can be interpreted as an estimate of the uncertainty in SAKF values due to uncertainties in the neutron spectra.

Table 3. ICRU Muscle SAKF for Calculated and Measured Reactor Neutron Spectra

Room	Distance to Core (cm)	Configuration	SAKF ( $10^{-10}$ rad cm <sup>2</sup> )		
			1-D	3-D	MEAS
1	100	Unshielded	19.4	20.3	16.8
2	100	Unshielded	13.8	14.4	10.9
1	100	30 cm H <sub>2</sub> O	27.3	34.4	
1	100	5 cm Pb	17.8	20.5	
1	100	5 cm Pb and exercise wheel	03.69	12.0	13.2
1	100	15 cm Pb	14.9	17.0	
1	100	15 cm Pb and cave	07.94	13.6	13.9
1	100	15 cm Pb and cylindrical phantom	02.11	02.85	4.51

Table 4 presents the reactor neutron SAKF's for three tissuelike materials. ICRU muscle, the generally accepted reference material for neutron dosimetry (7,8) is used as such here. ICRU tissue differs from ICRU muscle by a 2% lower hydrogen content (by weight), and the calculated kerma factors reflect this difference. DLC-31 tissue represents standard man composed of 11 elements, but the neutron SAKF values differ negligibly from those for ICRU muscle or ICRU tissue. A-150 is the tissue-equivalent plastic used for tissue-equivalent ion chamber construction.

Tissue-effective energies of the neutron spectra tabulated in Table 4 were determined in the same way as those of the gamma spectra. That is, tissue-effective spectrum energies were taken as the monoenergetic neutron energies giving the same tissue kerma factors as the spectra in question. The tissue-effective neutron energies display a decreasing trend with increasing free-in-air distance from the reactor (due to the increased importance of scattered neutrons), and an increasing trend for water-shielded configurations (due to a beam-hardening effect). Two phenomena are noteworthy: (a) The tissue-effective neutron energies are not equal to, nor do they correlate very well with, the average neutron energies given in Table 1. This finding emphasizes the fact that neutron spectra of complex shape cannot be represented well by any single energy descriptor. (b) The tissue-effective neutron energies are low at the two points with hydrogenous surrounds, i.e., pneumatic tubes and cylindrical phantom. Consideration of the shapes of the two neutron spectra plotted in Figure 1 clarifies this phenomenon. The spectra pertain to the reactor shielded with 15 cm of Pb, at a distance of 100 cm. One spectrum represents the case with no phantom present; the other spectrum is that at the center of the 18-cm-diameter cylindrical phantom. Within the phantom the total neutron flux below 0.01 MeV is 8.8 times the flux without the phantom, while the flux above 0.01 MeV is decreased by a factor of 5. It is the large low-energy component of the neutron spectrum within the phantom that causes such low tissue-effective neutron energy.

Table 4. Reactor Neutron Spectrum-Averaged Kerma Factors for Tissue

Room	Distance to Core (cm)	Configuration	MeV <sub>eff</sub>	SAKF (10 <sup>-10</sup> rad cm <sup>2</sup> )			
				Muscle* (ICRU)	Tissue <sup>†</sup> (ICRU)	Tissue (DLC-31) <sup>‡</sup>	A-150 Plastic <sup>§</sup>
1	50	Unshielded	0.8	19.8	19.6	19.6	20.0
	100	Unshielded	0.7	20.3	20.2	20.0	20.6
	200	Unshielded	0.6	17.6	17.4	17.4	17.8
	300	Unshielded	0.4	15.4	15.2	15.2	15.6
	400	Unshielded	0.4	13.6	13.4	13.4	13.7
	500	Unshielded	0.3	12.1	11.9	11.9	12.2
2	50	Unshielded	0.4	14.2	14.0	14.0	14.4
	100	Unshielded	0.4	14.4	14.2	14.2	14.5
	200	Unshielded	0.3	12.1	11.9	11.9	12.2
	300	Unshielded	0.2	10.6	10.5	10.5	10.7
NA	NA	Pneumatic tubes	0.04	3.83	3.70	3.75	3.87
1	100	7.5 cm H <sub>2</sub> O	1.0	23.7	23.4	23.4	24.1
	100	30 cm H <sub>2</sub> O	2.7	34.4	33.9	34.0	35.1
	100	5 cm Pb	0.8	20.5	20.2	20.2	20.4
	100	5 cm Pb and exercise wheel	0.3	12.0	11.8	11.8	12.0
	100	15 cm Pb	0.6	17.0	16.8	16.8	16.8
	100	15 cm Pb and cave	0.4	13.6	13.4	13.4	13.5
	100	15 cm Pb and cylindrical phantom	0.03	2.85	2.81	2.77	2.83
<u>Reference Spectra</u>							
		DLC-31 fission	0.8	20.4	20.1	20.1	20.4
		DLC-31 thermonuclear	0.6	18.1	17.8	17.8	18.3
		ENDF fission	1.16	28.3	27.9	27.9	28.4
		DLC-31 14 MeV	14.	64.6	63.9	63.2	67.4

\* Muscle (ICRU): 10.2% H, 12.3% C, 3.5% N, 72.9% O, 1.1% (Na + Mg + P + S + K + Ca) (from reference 1)

<sup>†</sup> Tissue (ICRU): 10.0% H, 14.9% C, 3.5% N, 71.6% O (from reference 1)

<sup>‡</sup> Tissue (DLC-31): 10% H, 24% C, 2.9% N, 60% O, 0.20% Na, 0.30% Mg, 1.1% P, 0.24% S, 0.20% K, 1.2% Ca, 0.20% Cl (from reference 5 of reference 4)

<sup>§</sup> A-150 plastic: 10.1% H, 77.6% C, 3.5% N, 5.2% O, 1.8% Ca, 1.7% F (from reference 1)

#### Reactor Neutron SAKF Ratios

SAKF results for the three ion chamber gas materials are shown in Table 5. For TE gas, all the reactor configurations can be represented by a single  $(K_T/K_{TE \text{ gas}})_N$  value of  $0.983 \pm 0.5\%$  (2 SD). For CO<sub>2</sub> and Ar, the SAKF ratios can be summarized as  $9.78 \pm 10\%$  and  $70.7 \pm 27\%$ , respectively. The variability among the CO<sub>2</sub> and Ar SAKF ratios indicates that individually tabulated values should be used for each reactor configuration.

Table 5. Reactor Neutron SAKF Ratios

Room	Distance to Core (cm)	Configuration	$(K_T/K_{TE \text{ gas}})_N^*$	$(K_T/K_{CO_2})$	$(K_T/K_{Ar})$
1	50	Unshielded	0.980	9.57	66.0
	100	Unshielded	0.979	9.50	64.3
	200	Unshielded	0.983	9.62	66.7
	300	Unshielded	0.981	9.68	67.5
	400	Unshielded	0.986	9.78	69.0
	500	Unshielded	0.984	9.84	70.3
2	50	Unshielded	0.979	9.59	66.0
	100	Unshielded	0.986	9.66	65.8
	200	Unshielded	0.984	9.68	67.2
	300	Unshielded	0.981	9.81	69.3
NA	NA	Pneumatic tubes	0.982	10.21	73.2
1	100	7.5 cm H <sub>2</sub> O	0.979	9.26	61.2
	100	30 cm H <sub>2</sub> O	0.983	8.49	55.5
	100	5 cm Pb	0.986	9.67	69.7
	100	5 cm Pb and exercise wheel	0.984	9.92	73.6
	100	15 cm Pb	0.983	10.18	83.7
	100	15 cm Pb and cave	0.986	10.38	92.5
	100	15 cm Pb and cylindrical phantom	0.986	11.00	91.1
	<u>Reference Spectra</u>				
		DLC-31 fission	0.986	9.86	76.7
		DLC-31 thermonuclear	0.989	6.24	50.7
		ENDF fission	0.983	9.53	65.2
		DLC-31 14 MeV	0.977	3.40	26.5

\* TE gas: 10.2% H, 45.6% C, 3.5% N, 40.7% O

The constancy of  $(K_T/K_{TE \text{ gas}})_N$  among the reactor configurations was to be expected, because this ratio varied only from 0.95 to 1.01 over the entire range of 37-energy groups. For the other neutron SAKF ratios, uncertainties can be estimated by again comparing results from calculated and measured spectra, as shown in Table 6. Although individual SAKF values have uncertainties of 2%-58%, SAKF ratios determined from calculated and measured spectra differ by only 1%-8%.



Table 6. SAKF Ratios for Calculated and Measured Neutron Spectra

Room	Distance to Core (cm)	Configuration	Neutron Spectrum		Difference (%)
			3-D	MEAS	
<u>K<sub>T</sub>/K<sub>Ar</sub></u>					
1	100	Unshielded	64.3	67.5	-5
2	100	Unshielded	65.8	67.7	-3
1	100	5 cm Pb and exercise wheel	73.6	74.6	-1
1	100	15 cm Pb and cave	92.5	91.4	+1
1	100	15 cm Pb and cylindrical phantom	91.1	84.3	+8
<u>K<sub>T</sub>/K<sub>CO<sub>2</sub></sub></u>					
1	100	Unshielded	9.50	9.66	-2
2	100	Unshielded	9.66	9.73	-1
1	100	5 cm Pb and exercise wheel	9.92	10.00	-1
1	100	15 cm Pb and cave	10.38	10.30	+1
1	100	15 cm Pb and cylindrical phantom	11.0	10.56	+4

## DISCUSSION

The gamma SAKF ratios for C and Mg (ion chamber wall materials) vary only slightly among the reactor configurations, and average values represent these quantities with fairly high precision. Historically it has been questioned (9,10) whether the AFRRI reactor gamma spectra can be approximated by cobalt-60 radiation (1.25 MeV). The present calculations confirm that this is nearly the case, since the average C and Mg SAKF ratios differ less than 4% from the values applicable to cobalt-60. However, in some configurations, a low-energy photon component in the reactor gamma spectra does cause C and Mg SAKF ratios to differ by up to 7.6% from corresponding values for cobalt-60.

The constancy of the neutron SAKF ratio for TE gas between the various reactor configurations was to be expected, because the compositions of TE gas and ICRU muscle match closely. For CO<sub>2</sub> and Ar, the neutron SAKF ratios are nearly constant for all free-in-air unshielded reactor configurations, but the ratios differ considerably (5%-40%) for more complex reactor configurations.

The differences between SAKF values derived from 3-D calculated neutron spectra and those derived from measured neutron spectra allow estimation of the uncertainties in the reported SAKF values arising from spectrum uncertainties. For ICRU muscle, the observed 2%-58% differences place a limit on dosimetric accuracy that can be obtained using a direct fluence-to-dose method. This emphasizes the importance of using ionization chambers for dose determination since the overall uncertainty of those chambers is about 10% (8). In this regard, the SAKF ratios for CO<sub>2</sub> and Ar differ by only 1%-8% between the 3-D calculated and measured neutron spectra. The improved precision for SAKF ratios over individual SAKF values is due to the similarity in energy response of the kerma factors for the different materials. This improved precision is indeed fortunate, because the SAKF ratios are required to evaluate paired ionization chamber response constants for reactor neutron and gamma dosimetry.

Considering the SAKF results for the reference spectra, it was apparent that for ICRU muscle and TE gas, the prompt gamma-ray fission source as well as the fission and thermonuclear sources fell within the range of values obtained for AFRRI reactor configurations. In particular, the 15-cm lead shield gave the same tissue-effective neutron energy as the thermonuclear source, and the 5-cm lead shield matched the fission source. However, these apparent similarities should be viewed with caution because, as pointed out above, no single energy descriptor can adequately represent a complex energy spectrum.

The results of this study demonstrate the need for further neutron spectrum calculations or measurements for AFRRI reactor configurations at depth in tissue-equivalent or anatomical phantoms. The large change in the neutron spectrum within the 18-cm-diameter phantom shows the importance of also studying phantoms of different sizes and shapes. The very low tissue-effective energy of the neutron spectrum within the phantom also suggests the need for more sophisticated dosimetric tools (such as tissue-equivalent proportional counters) to supplement the paired ionization chambers and to better quantitate the dose deposition process.

APPENDIX A.

Fortran Computer Program SPT

```

C** SPT
C   LATEST CORRECTION 17 AUG 82
C+
C   THIS PROGRAM WILL COMPUTE TWO SPECTRUM DEPENDENT FUNCTIONS:
C   A SPECTRUM WEIGHTED FUNCTION AND A SPECTRUM FOLDED FUNCTION,
C   AND THE ESTIMATED VARIATION OF EACH
C-
C   AUTHOR: KEN FERLIC CIRCA 1981 OR 82
C
C   THIS PROGRAM IS FOR EVALUATING THE INTEGRALS (BY SUMMATION)
C   NECESSARY FOR SPECTRUM AVERAGED QUANTITIES
C
C   NOTES
C   1. SPECTRUM INPUT DATA CAN BE A FROM AND BACK SPECTRUM
C   2. SPECTRUM INPUT DATA CAN BE LETHARGY, PHI(E)DE OR PHI(E)
C   3. THE DELTA SPECTRUM IS THE FACTIONAL CHANGE EXPECTED IN NEUTRON
C   POPULATION FOR A PARTICULAR ENERGY GROUP
C   4. THE DELTA FUNCTION IS THE FRACTIONAL CHANGE EXPECTED IN THE
C   FUNCTION PER ENERGY GROUP
C   5. ENERGY GROUP BOUNDS ARE THE UPPER BOUNDS
C   6. ENERGY GROUP 1 IS THE MAXIMUM ENERGY GROUP. I.E. GROUP 1 UPPER
C   BOUND IS 19.6 MEV
C
C   HIGHEST CONTROL STATEMENT IS 238
C   HIGHEST FORMAT STATEMENT IS 1217
C
C
C   BYTE FILE1(3C) 'FILE1=FLUX SPECTRUM FILE
C   BYTE FILE2(3C) 'FILE2=ENERGY GROUP FILE, UPPER BOUNDS
C   BYTE FILE3(3C) 'FILE3=FUNCTION FILE BY GROUP
C   BYTE FILE4(3C) 'FILE4=OUTPUT FILE
C   BYTE FILE5(3C) 'FILE5=DELTA SPECTRUM FILE
C   BYTE FILE6(3C) 'FILE6=DELTA FUNCTION FILE
C   DIMENSION PHIT(38) 'TOTAL INPUT FLUX
C   DIMENSION PHIF(38) 'TOTAL FRONT FLUX
C   DIMENSION PHIB(38) 'TOTAL BACK FLUX
C   DIMENSION IGROUP(38) 'GROUP NUMBER
C   INTEGER NROW 'NUMBER OF GROUPS NUMBER OF INPUT ROWS
C   INTEGER ICOL 'NUMBER OF COLUMNS IN INPUT DATA
C   INTEGER ICNT 'COUNTER OF FOR FILE NAMES
C   INTEGER NSPT 'TYPE OF FLUX INPUT IE ENERGY,LETHARGY
C   INTEGER NTYPE 'TYPE OF INPUT SPECTRUM TOTAL VS FRONT + BACK
C   DIMENSION ENGP(38) 'ENERGY GROUP UPPER BOUNDS
C   DIMENSION FNCT(38) 'FUNCTION GROUPS
C   DIMENSION DE(38) 'CHANGE IN ENERGY
C   DIMENSION DU(38) 'CHANGE IN LETHARGY
C   REAL DUBWI 'DESIRED UPPER BOUND WEIGHTING INTEGRAL
C   REAL DLBWI 'DESIREES LOWER BOUND WEIGHTING INTEGRAL
C   REAL DUBNI 'DESIRED UPPER BOUND NORMALIZING INTEGRAL
C   REAL DLBNI 'DESIRED LOWER BOUND NORMALIZING INTEGRAL
C   INTEGER IUBCWI 'UPPER BOUND GROUP WEIGHTING INTEGRAL
C   REAL UBFWI 'UPPER BOUND FRACTION WEIGHTING INTEGRAL
C   INTEGER IUBFCW 'UPPER BOUND FRACTIONAL GROUP WEIGHTING INTEP
C   INTEGER IUBGNI 'UPPER BOUND GROUP NORMALIZING INTEGRAL
C   REAL UBFNI 'UPPER BOUND FRACTION NORMALIZING INTEGRAL
C   INTEGER IUBFGN 'UPPER BOUND FRACTIONAL GROUP NORMALIZING INT
C   INTEGER ILBFWI 'LOWER BOUND GROUP WEIGHTING INTEGRAL
C   REAL LBFWI 'LOWER BOUND FRACTION WEIGHTING INTEGRAL
C   INTEGER ILBFCW 'LOWER BOUND FRACTIONAL GROUP WEIGHTING INTEP
C   INTEGER ILBFGN 'LOWER BOUND FRACTIONAL GROUP NORMALIZING INT
C   REAL LBFNI 'LOWER BOUND FRACTION NORMALIZING INTEGRAL

```

INTEGER ILBGN1	!LOWER BOUND GROUP NORMALIZING INTEGRAL
REAL WINT	!INTEGRAL OF THE WEIGHTING INTERGRAL
REAL NINT	!INTEGRAL OF THE NORMALIZING INTEGRAL
REAL PNCFF	!EFFECTIVE VALUE OF FUNCTION
INTEGER NROW1	!ROWS IN INPUT SPECTRUM FILE
INTEGER NROW2	!ROWS IN INPUT ENEGRY GROUP FILE
INTEGER NROW3	!ROWS IN INPUT FUNCTION GROUP FILE
INTEGER NROW5	!ROWS IN INPUT DELTA SPECTRUM FILE
INTEGER NROW6	!ROWS IN INPUT DELTA FUNCTION FILE
DIMENSION FRCTW(38)	!FRACTION OF WEIGHTING INTEGRAL FOR GROUP I
DIMENSION FRCTN(38)	!FRACTION OF NORMALIZING INTEGRAL FOR GROUP I
DIMENSION DELTA(38)	!DE OR DU IN INTEGRAL FOR GROUP I
REAL UTAIL	!UPPER TAIL OF INTEGRAL BETWEEN GROUPS
REAL LTAIL	!LOWER TAIL OF INTEGRAL BETWEEN GROUPS
INTEGER SAF	!CONTROL FOR SPECTRUM AVERAGED FUNCTIONS
INTEGER VSAF	!CONTROL FOR VARIATION OF SPECTRUM AVERAGED
INTEGER SFF	!CONTROL FOR SPECTRUM FOLDED FUNCTION
INTEGER VSFF	!CONTROL FOR VARIATION OF SPECTRUM FOLDED
INTEGER INPUT1	!DELTA (VARIATION) FILES CONTROL CHARACTER
INTEGER INPUT2	!BOUNDS ON NORMALIZING INTEGRAL CONTROL
INTEGER INPUT3	!TEMPORARY NORMALIZING INTEGRAL CONTROL
DIMENSION DFF(38)	!DELTA FUNCTION ENTRY
DIMENSION DSF(38)	!DELTA SPECTRUM ENTRY
DIMENSION PHIENR(38)	!PHI(E) FOR EACH GROUP
REAL UBFEW	!FRACTION OF ENERGY UPPER END WGT INT
REAL UBFEN	!FRACTION OF ENERGY UPPER END NOR INT
REAL LBFWE	!FRACTION OF ENERGY LOWER END WGT INT
REAL LBFEN	!FRACTION OF ENERGY LOWER END NOR INT
DIMENSION DEW(38)	!DELTA E FOR WGT INT IN VARIATION CALCULATION
DIMENSION DEN(38)	!DELAT E FOR NOR INT IN VARIATION CALCULATION
DIMENSION PWPFI(38)	!PARTIAL WGT WITH RESPECT TO PHI
DIMENSION PWFNT(38)	!PARTIAL WGT WITH RESPECT TO THE FUNCTION
DIMENSION PWSUM(38)	!SUM OF PARTIALS WITH RESP TO PHI AND FUNCT
REAL VFFNCT	!VARIATION OF FOLDED FUNCTION
DIMENSION TERM1(38)	!FIRST TERM IN CALCULATION OF VAR OF WGT FNCT
DIMENSION TERM2(38)	!SECOND TERM IN CALCUL OF VAR OF WGT FNCT
DIMENSION TERM3(38)	!THIRD TERM IN CALCUL OF VAR OF WGT FNCT
DIMENSION PWFPHI(38)	!PARTIAL OF WGT FNCT WITH RESPECT TO PHI SCF
DIMENSION PWFNT(38)	!PARTIAL OF WGT FNCT WITH RESPECT TO FNT SCF
REAL VWFNT	!VARIATION OF WEIGHTED FUNCTION

C  
C  
C  
COMMON STATEMENTS FOR SUBROUTINES UPBND AND LWBND

COMMON IXGP,XDUB,XE(38),IXUBG,IXUBFG,XUBF  
COMMON XDLB,IXLBG,IXLBFG,XLBF,XUBFE,XLEFE

C  
C  
C  
DETERMINATION OF CALCULATIONS TO BE PERFORMED

TYPE 1200  
1200   FORMAT(' DO YOU WANT A SPECTRUM AVERAGED FUNCTION? YES=1,NO=0  
1   OR CR')  
      ACCEPT 1201,SAF  
1201   FORMAT(I3)  
      IF(SAF .EQ. 0)GO TO 200  
      TYPE 1202  
1202   FORMAT(' DO YOU WANT THE ESTIMATED VARIATION? YES=1, NO=0 OR CR')  
      ACCEPT 1201,VSAF  
200   CCONTINUE

```

1203      TYPE 1203
          FORMAT(' DO YOU WANT A SPECTRUM FOLDED FUNCTION? YES=1,NO=0 OR CR')
          ACCEPT 1201,SFF
          IF(SFF .EQ. 0)GO TO 201
          TYPE 1204
1204      FORMAT(' DO YOU WANT THE ESTIMATED VARIATION? YES=1, NO=0 OR CR')
          ACCEPT 1201,VSFF
201        CONTINUE
          IF(SAF .NE. SFF)GO TO 203
          IF(SAF .EQ. 0)GO TO 202
          GO TO 203
202        TYPE 1205
1205      FORMAT(' WHAT DO YOU WANT??? BYE, BYE')
          GO TO 140
203        CONTINUE

C
C      PROGRAM CONTROL FOR CALCULATIONS, DETERMINATION OF ACTUAL INPUT DATA
C
C      INPUT1  DELTA FILES INPUT,
C      INPUT2  BOUNDS ON NORMALIZING INTEGRAL  INPUT
C

          IF(SAF .EQ. 0)GO TO 204
          INPUT1=0
          INPUT2=1
          IF(VSAF .EQ.C)GO TO 204
          INPUT1=1
204        CONTINUE
          IF(SFF .EQ. 0)GO TO 205
          INPUT1=C
          INPUT3=C
          IF(VSFF .EQ.C)GO TO 205
          INPUT1=1
205        CONTINUE
          IF(INPUT2 .EQ. INPUT3)GO TO 229
          INPUT2=1
229        CONTINUE

C
C      IDENTIFY NUMEER OF GROUPS
C

          TYPE 1116
1116      FORMAT(' WHAT IS THE NUMBER OF GROUPS IN SPECTRUM:<I3>')
          ACCEPT 1006,NROW

C
C      SET LOW BOUND ON LOWEST ENERGY GROUP
C

          IF(NROW .EQ. 37)GO TO 119
          IF(NROW .EQ. 21)GO TO 120
          TYPE 1120
1120      FORMAT(' WHAT IS LOWER BOUND (IN EV) ON THE LOWEST ENERGY'
                ' GROUP?<E10.4>')
          ACCEPT 1121, ENGP(NROW+1)
1121      FORMAT(E10.8)
          GO TO 121
119      ENGP(38)=1.CE-5      'IN EV
          GO TO 121

```

```

120      ENGP(22)=1.OE+4      'IN EV
121      CONTINUE

C
C      FILE1 NAME: SPECTRUM FILE
C

      TYPE 1000
1000      FORMAT(' ENERGY SPECTRUM FILE NAME <FILENAMEX.TYP>:')
      ACCEPT 1001,ICNT,FILE1
1001      FORMAT(Q,30A1)
      FILE1(ICNT+1)=0
      TYPE 1005
1005      FORMAT(' SPECTRUM INPUT: FRONT + BACK = 0, TOTAL = 1')
      ACCEPT 1006, NTYPE
1006      FORMAT(I3)
      TYPE 1115
1115      FORMAT(' IS SEPCTRUM INPUT: PHI(U)=1,PHI(E)DE=C,PHI(E)=-1')
      ACCEPT 1006,NSPT

C
C      FILE2 NAME: ENERGY GROUP UPPER BOUND FILE
C

      TYPE 1003
1003      FORMAT(' ENTER ENERGY GROUP (UPPER BOUND) FILE: <FILENAMEX.TYP>')
      ACCEPT 1001,ICNT,FILE2
      FILE2(ICNT+1)=0

C
C      FILE3 NAME: FUNCTION GROUP FILE
C

      TYPE 1004
1004      FORMAT(' ENTER FUNCTION GROUP FILE: <FILENAMEX.TYP>')
      ACCEPT 1001,ICNT,FILE3
      FILE3(ICNT+1)=0

C
C      FILE4 NAME: OUTPUT FILE NAME
C

      TYPE 1198
1198      FORMAT(' ENTER OUTPUT FILE NAME:<FILENAMEX.TYP>')
      ACCEPT 1001,INCT,FILE4
      FILE4(INCT+1)=0

C
C      FILE5 NAME: DELTA SPECTRUM FILE
C

      IF(INPUT1 .EQ. C)GO TO 206
      TYPE 1206
1206      FORMAT(' ENTER DELTA SPECTRUM FILE NAME <FILENAMEX.TYP>:')
      ACCEPT 1001,INCT,FILE5
      FILE5(INCT+1)=0

C
C      FILE6 NAME: DELTA FUNCTION FILE
C

      TYPE 1207

```

```

1207  FORMAT(' ENTER DELTA FUNCTION FILE NAME <FILENAMEX.TYP>:')
      ACCEPT 1001,INCT,FILE6
      FILE6(INCT+1)=0
2006  CONTINUE

C
C      EXTRACT DATA FROM SPECTRUM FILE: FILE1
C

      OPEN(UNIT=1,NAME=FILE1,TYPE='OLD')
      READ(1,1007) ICOL,NROW1
1007  FORMAT(2I4)
      IF(NROW1 .NE. NROW)GO TO 112
      IF(NTYPE .EQ. C)GO TO 100
      DO 101 I=1,NROW
      READ(1,1008) IGROUP(I),PHIT(I)
1008  FORMAT(I3,E12.4)
1001  CONTINUE
      GO TO 102
100  DO 103 I=1,NROW
      READ(1,1009)IGROUP(I),PHIF(I),PHIB(I)
1009  FORMAT(I3,2E12.4)
1003  CONTINUE
1002  CONTINUE
      CLOSE(UNIT=1)

C
C      EXTRACT DATA FROM ENERGY GROUP FILE
C

      OPEN(UNIT=1,NAME=FILE2,TYPE='OLD')
      READ(1,1007)ICOL,NROW2
      IF(NROW2 .NE. NROW)GO TO 114
      DO 104 I=1,NROW
      READ(1,1006) IGRUP(I),ENGP(I)
1004  CONTINUE
      CLOSE(UNIT=1)

C
C      EXTRACT DATA FROM FUNCTION FILE:FILE3
C

      OPEN(UNIT=1,NAME=FILE3,TYPE='OLD')
      READ(1,1007),ICOL,NROW3
      IF(NROW3 .NE. NROW)GO TO 115
      DO 105 I=1,NROW
      READ(1,1008), IGROUP(I),FNCT(I)
1005  CONTINUE
      CLOSE(UNIT=1)

C
C      EXTRACT DATA FROM DELTA SPECTRUM FILE: FILE4
C

      IF(INPUT1 .EQ. C)GO TO 207
      OPEN(UNIT=1,NAME=FILE5,TYPE='OLD')
      READ(1,1007),ICOL,NROW5
      IF(NROW5 .NE. NROW)GO TO 208
      DO 209 I=1,NROW
      READ(1,1008),IGROUP(I),DSF(I)
2009  CONTINUE
      CLOSE(UNIT=1)

```



```

C
C   EXTRACT DATA FROM DELTA FUNCTION FILE:FILE6
C
      OPEN(UNIT=1,NAME=FILE6,TYPE='OLD')
      READ(1,1007),ICOL,NROW6
      IF(NROW6 .NE. NROW)GO TO 210
      DO 211 I=1,NROW
      READ(1,1008),IGROUP(I),DFF(I)
211    CONTINUE
      CLOSE(UNIT=1)
207    CONTINUE
      GO TO 141

C
C   CHECK FOR PROPER NUMBER OF GROUPS IN EACH INPUT FILE; NEGATIVE ANSWER
C
      TYPE 1117,NROW1
      GO TO 113
      TYPE 1117,NROW2
      GO TO 113
      TYPE 1117,NROW3
      GO TO 113
      TYPE 1117,NROW5
      GO TO 113
      TYPE 1117,NROW6
      FORMAT(' ACTUAL GROUPS IN FILE',I3)
      TYPE 1199,NROW
      FORMAT(' DOES NOT EQUAL IDENTIFIED SPECTRUM GROUPS:',I3)
      CLOSE(UNIT=1)
      GO TO 140

C
C   CALCULATE TOTAL FLUX IF FRONT AND BACK
C
      IF(NTYPE .EQ. 1)GO TO 106
      DO 107 I=1, NROW
      PHIT(I)=PHIF(I)+PHIB(I)
107    CONTINUE
106    CONTINUE

C
C   CALCULATE DU OR DE FOR THE SPECTRUM
C
      OLD LINE      IF(NSPT) 116,117,118

C
C   CHANGE IN LETHARGY/ENERGY
C
      DO 108 I=1,NROW
      DU(I)=LOG(ENGF(I)/ENGP(I+1))
108    CONTINUE
      OLD LINE      GO TO 117
      DO 109 I=1,NROW
      DE(I)=ENGF(I)-ENGP(I+1)
109    CONTINUE
117    CONTINUE

```

```

C
C      ACCEPT BOUNDS ON WEIGHTING AND NORMALIZING INTEGRAL
C
      TYPE 1010
1010  FORMAT(' WHAT IS UPPER BOUND OF WEIGHTING INTEGRAL IN EV:'
      1 '<E10.4>')
      TYPE 1122
1122  FORMAT(' NEUTRON 37 GROUP MAX IS 19.6E+6 EV; PHOTON 21 GROUP MAX'
      1 'IS 14.0E+6 EV')
      ACCEPT 1011,DUBW1
1011  FORMAT(E10.4)
      TYPE 1012
1012  FORMAT(' WHAT IS LOWER BOUND OF WEIGHTING INTEGRAL IN EV:'
      1 '<E10.4>')
      TYPE 1123
1123  FORMAT(' NEUTRON 37 GROUP MIN IS 1.0E-5 EV; PHOTON 21 GROUP MAX'
      1 'IS 1.0E+4 EV')
      ACCEPT 1011,DLBW1

C
C      ACCEPT BOUNDS ON NORMALIZING INTEGRAL
C
      IF(INPUT2 .EQ. C)GO TO 212
      TYPE 1013
1013  FORMAT(' WHAT IS UPPER BOUND ON NORMALIZING INTEGRAL IN EV:'
      1 '<E10.4>')
      TYPE 1122
      ACCEPT 1011,DUBN1
      TYPE 1014
1014  FORMAT(' WHAT IS LOWER BOUND ON NORMALIZING INTEGRAL IN EV:'
      1 '<E10.4>')
      TYPE 1123
      ACCEPT 1011,DLBN1
212  CONTINUE

C
C      SET UPPER BOUND ON WEIGHTING INTEGRAL
C
      IXGP=NRCW+1
      XDUB=DUBW1
      DO 151 I=1, NROW+1
      XE(I)=ENGP(I)
151  CONTINUE
      CALL UPBND
      IUBGWI=IXUBG
      UEPWI=XUBF
      IUBFGW=IXUBFG
      UEPFW=XUBFE

C
C      SET UPPER BOUND ON NORMALIZING INTEGRAL
C
      IF(INPUT2 .EQ. C)GO TO 213
      XDUB=DUBN1
      CALL UPENI
      IUBFGN=IXUBFG
      UBFNI=XUBF
      IUBGNI=IXUBG
      UBFEN=XUBFE

```

```

213      CONTINUE

C
C      SET LOWER BOUND WEIGHTING INTEGRAL
C

      XDLB=DLBWI
      CALL LOWBND
      ILBGWI=IXLBG
      LBFWI=XLBF
      ILBFGW=IXLBFG
      LBFEW=XLBFEL
      LBFEW=XLBFEL

C
C      SET LOWER BOUND ON NORMALIZING INTEGRAL
C

      IF(INPUT2 .EQ. C)GO TO 214
      XDLB=DLENI
      CALL LOWEND
      ILBFGN=IXLBFG
      LBFNI=XLBF
      ILBENI=IXLBG
      LBFEN=XLBFEL
214      CONTINUE

C
C      EVALUATION OF WEIGHTING INTEGRAL
C

      DO 110 I=1,NROW
      FRCTW(I)=C.C
      FRCTN(I)=C.C
110      CONTINUE

C
C      DETERMINE DELTA TERMS FOR INTEGRALS I.E. LE OR DU
C      PLACE ALL DATA IN THE FORM OF PHI/E, IRREGARDLESS OF INPUT
C

      IF(NSPT) 122,123,124
122      DO 125 I=1,NROW
      DELTA(I)=DE(I)
      PHIENR(I)=PHIT(I)
125      CONTINUE
      GO TO 126
123      DO 127 I=1,NROW
      DELTA(I)=1.0
      PHIENR(I)=PHIT(I)/DE(I)
127      CONTINUE
      GO TO 126
124      DO 128 I=1,NROW
      DELTA(I)=DU(I)
      PHIENR(I)=PHIT(I)*DU(I)/DE(I)
128      CONTINUE

C
C      EVALUATION OF WEIGHTING/FOLDING INTEGRAL
C

126      SUM=C.C
      DO 150 I=1,ILBGWI,ILBENI

```

```

FRCTW(I)=PHIT(I)*DELTA(I)*FNCT(I)
SUM=SUM+FRCTW(I)
150 CONTINUE
UTAIL=PHIT(IUBFGW)*DELTA(IUBFGW)*FNCT(IUBFGW)*UBFWI
LTAIL=PHIT(ILBFGW)*DELTA(ILBFGW)*FNCT(ILBFGW)*LBFWI
IF(IUBGWI .EQ. IUBFGW)GO TO 230
FRCTW(IUBFGW)=UTAIL
230 IF(ILBGWI .EQ. ILBFGW)GO TO 231
FRCTW(ILBFGW)=LTAIL
231 WINT=SUM+UTAIL+LTAIL

C
C EVALUATION OF NORMALIZING INTEGRAL
C

IF(INPUT2 .EQ. 0)GO TO 215
SUM=0.0
DO 111 I=IUEGNI,ILBONI
FRCTN(I)=PHIT(I)*DELTA(I)
SUM=SUM+FRCTN(I)
111 CONTINUE
UTAIL=PHIT(IUEFGN)*DELTA(IUEFGN)*UEFNI
LTAIL=PHIT(ILBFGN)*DELTA(ILBFGN)*LEFNI
IF(IUBGNI .EQ. IUEFGN)GO TO 232
FRCTN(IUEFGN)=UTAIL
232 IF(ILBONI .EQ. ILEFGN)GO TO 233
FRCTN(ILBFGN)=LTAIL
233 NINT=SUM+UTAIL+LTAIL

C
C EVALUATE EFFECTIVE FUNCTION
C

FNCEFF=WINT/NINT
215 CONTINUE

C
C SET OF DE FOR DELTA E IN THE FOLDED FUNCTION VARIATION EQUATION
C

IF(INPUT1 .EQ. 0)GO TO 216
IC=IUBFGW-1
DO 217,I=1,IC
DEW(I)=0.0
217 CONTINUE
IC=(NROW+1)-ILBFGW
DO 218 I=1,IC
L=(NROW+1)-I
DEW(L)=0.0
218 CONTINUE
DO 219 I=IUBFGW,ILBFGW
DEW(I)=DE(I)
219 CONTINUE
IF(IUBFGW .EQ. IUEGWI)GO TO 236
DEW(IUBFGW)=DEW(IUBFGW)*UEFEW
236 IF(ILBFGW .EQ. ILPGWI)GO TO 237
DEW(ILBFGW)=DEW(ILEFGW)*LEFEW
237 CONTINUE

C
C COMPUTE ESTIMATED VARIATION IN THE FOLDED FUNCTION
C

```

```

SUM=0.0
DO 220 I=1,NROW
PWPFI(I)=(FNCT(I)*DSF(I)*PHIENR(I)*DEW(I))**2
PWFNT(I)=(PHIENR(I)*DFF(I)*FNCT(I)*DEW(I))**2
PWSUM(I)=PWPFI(I)+PWFNT(I)
SUM=PWSUM(I)+SUM
220 CONTINUE
VFFNCT=SUM**0.5

C
C SET UP OF DE FOR DELTA E IN THE NORMALIZING INTEGRAL PORTION
C OF THE EXPECTED VARIATION IN THE WEIGHTED FUNCTION
C

IF(INPUT2 .EQ. 0)GO TO 216
IC=IUBFGN-1
DO 228 I=1,IC
DEN(I)=0.0
228 CONTINUE
IC=NROW-ILBFGN
DO 221 I=1,IC
L=(NROW+1)-I
DEN(L)=0.0
221 CONTINUE
DO 222 I=IUBFGN,ILBFGN
DEN(I)=DE(I)
222 CONTINUE
IF(IUBFGN .EQ. IUBGNI)GO TO 234
DEN(IUBFGN)=DEN(IUBFGN)*UBFEN
234 IF(ILBFGN .EQ. ILBGNI)GO TO 235
DEN(ILBFGN)=DEN(ILBFGN)*LBFEN
235 CONTINUE

C
C COMPUTE EXPECTED VARIATION IN WEIGHTED FUNCTION
C

SUM=0.0
DO 223 I=1, NROW
TERM1(I)=FNCT(I)*DEW(I)/NINT
TERM2(I)=WINT*DEN(I)/(NINT**2)
XXX=(TERM1(I)-TERM2(I))
PWPFI(I)=(XXX*PHIENR(I)*DSF(I))**2
TERM3(I)=PHIENR(I)*DEW(I)/NINT
PWFNT(I)=(TERM3(I)*FNCT(I)*DFF(I))**2
SUM=PWPFI(I)+PWFNT(I)+SUM
223 CONTINUE
VWFNT=SUM**0.5
216 CONTINUE

C
C OPEN OUTPUT FILE
C

OPEN(UNIT=1,NAME=FILE4,TYPE='NEW')

C
C OUTPUT ALL DATA
C

WRITE(1,1124)

```

```

1124 TYPE 1124
      FORMAT(' GROUP ENERGY      PHI      DELETA      FUNCTION ')
      DO 129 I=1,NROW
      WRITE(1,1125)I,ENGP(I),PHIT(I),DELTA(I),FNCT(I)
      TYPE 1125, I,ENGP(I),PHIT(I),DELTA(I),FNCT(I)
1125 FORMAT(I5,4E11.4)
129  CONTINUE
      WRITE(1,1126)
      TYPE 1126
1126 FORMAT(' GROUP ENERGY FRACTION NUMERATOR FRACTION DENOMINAT'
1      'OR')
      DO 130 I=1,NROW
      WRITE(1,1127) IGROUP(I),ENGP(I),FRCTW(I),FRCTN(I)
      TYPE 1127,IGROUP(I),ENGP(I),FRCTW(I),FRCTN(I)
1127 FORMAT(I5,E11.4,8X,E11.4,12X,E11.4)
130  CONTINUE
      TYPE 1128
      WRITE(1,1128)
1128 FORMAT(2CX,' NUMERATOR INTEGRAL DENOMINATOR INTEGRAL')
      WRITE(1,1129) IUBGWI,IUBGNI
      TYPE 1129, IUBGWI,IUBGNI
1129 FORMAT(' UPPER BOUND GROUP ',10X,I3,18X,I3)
      WRITE(1,1130) ILBGWI,ILBGNI
      TYPE 1130,ILBGWI,ILBGNI
1130 FORMAT(' LOWER BOUND GROUP ',10X,I3,18X,I3)
      WRITE(1,1131)IUBFGW,IUBFGN
      TYPE 1131,IUBFGW,IUBFGN
1131 FORMAT(' FRACTION GROUP UB ',10X,I3,18X,I3)
      WRITE(1,1132)ILBFGW,ILBFGN
      TYPE 1132, ILBFGW,ILBFGN
1132 FORMAT(' FRACTION GROUP LB ',10X,I3,18X,I3)
      WRITE(1,1133)UBFWI,UBFNI
      TYPE 1133,UBFWI,UBFNI
1133 FORMAT(' UPPER BOUND FRACTION',9X,E11.3,11X,E11.3)
      TYPE 1134, LBFWI,LBFNI
      WRITE(1,1134) LBFWI,LBFNI
1134 FORMAT(' LOWER BOUND FRACTION',9X,E11.3,11X,E11.3)
      TYPE 1135, DUBWI,DUBNI
      WRITE(1,1135) DUBWI,DUBNI
1135 FORMAT(' UPPER BOUND ',16X,E11.3,11X,E11.3)
      TYPE 1136, DLBWI,DLBNI
      WRITE(1,1136)DLBWI,DLBNI
1136 FORMAT(' LOWER BOUND',16X,E11.3,11X,E11.3)
      TYPE 1137, WINT,NINT
      WRITE(1,1137) WINT,NINT
1137 FORMAT(' INTEGRAL ',20X,E11.3,11X,E11.3)
      TYPE 1138, FNCEFF
      WRITE(1,1138) FNCEFF
1138 FORMAT(' WEIGHTED FUNCTION ',17X,E11.3)
      TYPE 1208,VFFNCT
      WRITE(1,1208),VFFNCT
1208 FORMAT(' VARIATION ON FOLDED FUNCTION ',9X,E11.3)
      TYPE 1209, VWFNT
      WRITE(1,1209),VWFNT
1209 FORMAT(' VARIATION OF WEIGHTED FUNCTION ',7X,E11.3)
      TYPE 1210
      WRITE(1,1210)
1210 FORMAT(' GROUP DELTA FNCT DELTA SPECT PHIENR')
      DO 224 I=1,NROW
      TYPE 1211,IGROUP(I),DFF(I),DSF(I),PHIENR(I)
      WRITE(1,1211),IGROUP(I),DFF(I),DSF(I),PHIENR(I)
1211 FORMAT(I5,E11.4,8X,E11.4,12X,E11.4)

```

```

224  CONTINUE
      TYPE 1212
      WRITE(1,1212)
1212  FORMAT(' GROUP          DEW          PWPFI          PWFNT')
      DO 225 I=1,NROW
      TYPE 1213,IGROUP(I),DEW(I),PWPFI(I),PWFNT(I)
      WRITE(1,1213),IGROUP(I),DEW(I),PWPFI(I),PWFNT(I)
1213  FORMAT(I5,E11.4,8X,E11.4,12X,E11.4)
225  CONTINUE
      TYPE 1214
      WRITE(1,1214)
1214  FORMAT(' GROUP          TERM1          TERM2          TERM3')
      DO 226 I=1,NROW
      TYPE 1215,IGROUP(I),TERM1(I),TERM2(I),TERM3(I)
      WRITE(1,1215),IGROUP(I),TERM1(I),TERM2(I),TERM3(I)
1215  FORMAT(I5,E11.4,8X,E11.4,12X,E11.4)
226  CONTINUE
      TYPE 1216
      WRITE(1,1216)
1216  FORMAT(' GROUP          DEN          PWFPFI          PWFFNT')
      DO 227 I=1,NROW
      TYPE 1217,IGROUP(I),DEN(I),PWFPFI(I),PWFFNT(I)
      WRITE(1,1217),IGROUP(I),DEN(I),PWFPFI(I),PWFFNT(I)
1217  FORMAT(I5,E11.4,8X,E11.4,12X,E11.4)
227  CONTINUE
      CLOSE(UNIT=1)
140  CONTINUE
      STOP
      END

C
C  SUBROUTINE UPBND
C

      SUBROUTINE UPBND

C
C  THIS SUBROUTINE CALCULATES THE UPPER BOUND ON INTEGRALS IN WHICH
C  THE INPUT DATA IS IN GROUPS BUT THE LIMIT IS BETWEEN THE
C  BOUNDS OF A GROUP
C

      COMMON IGP,DUB,E(38),IUBG,IUBFG,UBF
      COMMON DLB,ILBG,ILBFG,XLBF,UBFE,XLBFE

C
C  IGP = NUMBER OF GROUPS
C  DUB = DESIRED UPPER BOUND
C  E(38) = ENERGY GROUP SPECTRUM (UPPER ENERGY BOUNDS)
C  IUBG = UPPER BOUND GROUP
C  IUBFG = UPPER BOUND FRACTIONAL GROUP
C  UBF = UPPER BOUND FRACTION OF GROUP FOR PHI*DE OR PHI*DU
C  UBFE = UPPER BOUND FRACTION OF ENERGY
C  DLB = DESIRED LOWER BOUND
C  ILBG = LOWER BOUND GROUP
C  ILBFG = LOWER BOUND FRACTIONAL GROUP
C  XLBF = LOWER BOUND FRACTION OF GROUP FOR PHI*DE OR PHI*DU
C  XLBFE = LOWER BOUND FRACTION OF ENERGY

C
C  LOOK TO SEE IF UPPER BOUND LIES ON A BOUNDARY
C

```

```

      ISET=0
      DO 1 I=1,IGP
      ISET=ISET+1
      IF(DUB .EQ. E(I)) GO TO 100
1      CONTINUE
      GO TO 101
100     IUBG=ISET
      IUBFG=ISET
      UBF=0.0
      GO TO 105

C
C      IF UPPER BOUND LIES BETWEEN GROUPS, FIND FRACTION OF GROUP
C

101     ISET=0
      DC 103 I=1,IGP+1
      ISET=ISET+1
      IF(DUB .GT. E(I)) GO TO 104
103     CONTINUE
104     IUBG=ISET
      IUBFG=ISET-1
      DELTAE=E(ISET-1)-E(ISET)

C
C      NOTE: E(ISET-1) IS THE HIGHER ENERGY
C

      PARTE=DUB-E(ISET)
      X1=E(ISET-1)
      X2=E(ISET)
      XDELTA=ALOG(X1)-ALOG(X2)
      XPART=ALOG(DUB)-ALOG(X2)
      UBF=SQRT((XPART/XDELTA)**2)
      UBFE=PARTE/DELTAE

C
C      NOTE: IF DUB=E(ISET) THEN DUB-E(ISET)=C AND UBF=0
C

105     TYPE 1002
1002     FORMAT(' TEMP AT SUBROUTINE FORMAT 1002')
      TYPE 1000
1000     FORMAT(' IUBG,IUBFG,UBF,DELTAE,PORTE')
      TYPE 1001,IUBG,IUBFG,UBF,DELTAE,PORTE
1001     FORMAT(2I5,3E12.4)
      RETURN
      END

C
C      SUBROUTINE LOWBND
C

      SUBROUTINE LOWBND

C
C      THIS SUBROUTINE IS FOR CALCULATING THE LOWER BOUND ON INTEGRALS
C      WHERE THE INPUT DATA IS IN GROUPS AND THE CHOSEN BOUND IS BETWEEN
C      THE BOUNDS OF A GROUP
C

      COMMON IGP,DUB,E(38),IUBG,IUBFG,UBF
      COMMON DLB,ILBG,ILBFG,ILBF,UBFE,XLEFE

```



```

C
C IGP = NUMBER OF GROUPS
C DUB = DESIRED UPPER BOUND
C E(38) = ENERGY GROUP SPECTRUM (UPPER ENERGY BOUNDS)
C IUBG = UPPER BOUND GROUP
C IUBFG = UPPER BOUND FRACTIONAL GROUP
C UBF = UPPER BOUND FRACTION OF GROUP FOR PHI*TE OR PHI*DU
C UBFE=UPPER BOUND FRACTION OF ENERGY
C DLB = DESIRED LOWER BOUND
C ILBG = LOWER BOUND GROUP
C ILBFG = LOWER BOUND FRACTIONAL GROUP
C XLBF = LOWER BOUND FRACTION OF GROUP FOR PHI*DE OR PHI*DU
C XLBFE=LOWER BOUND FRACTION OF ENERGY
C
C CHECK TO SEE IF THE LOWER BOUNDRY LIES ON A BOUNDRY
C
C
C ISET=0
C DO 1 I=1,IGP+1
C ISET=ISET+1
C IF(DLB .EQ. E(I))GO TO 100
1 CONTINUE
C GO TO 101
100 ILBG=ISET-1
C ILBFG=ISET-1
C XLBF=0.0
C GO TO 105
C
C IF LOWER BOUND LIES IN A BOUNDRY OF A GROUP FIND THE FRACTION OF
C OF THAT GROUP
C
C
101 ISET=0
C DO 103 I=1, IGP
C IF(DLB .GT. E(I))GO TO 104
C ISET=ISET+1
103 CONTINUE
104 ILEG=ISET-1
C ILBFG=ISET
C DELTAE=E(ISET-1)-E(ISET)
C PARTE=E(ISET-1)-DLB
C X1=E(ISET-1)
C X2=E(ISET)
C XDELTA=ALOG(X1)-ALOG(X2)
C XPART=ALOG(X1)-ALOG(DLB)
C XLBF=SQRT((XPART/XDELTA)**2)
C XLBFE=PARTE/DELTAE
105 TYPE 1002
1002 FORMAT(' TEMP FROM SUBROUTINE LOWEND FCRMAT 1002')
C TYPE 1000
1000 FORMAT(' ILBG,ILBFG,XLBF,DELTAE,PART')
C TYPE 1001, ILBG,ILBFG,XLBF,DELTAE,PART
1001 FORMAT(2I5,3E12.4)
C RETURN
C END

```

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